

Diethylene glycol diethyl ether
112-36-7 | DTXSID3025047

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.50×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.92×10^{-1}

Confidence level: 8.15×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Diethylene glycol diethyl ether

Measured: 2.68×10^{-11}

Predicted: 2.50×10^{-11}

Image not found

3-Methoxybutan-1-ol

Measured: 2.36×10^{-11}

Predicted: 2.52×10^{-11}

Image not found

2-Butoxyethanol

Measured: 1.86×10^{-11}

Predicted: 2.09×10^{-11}

Image not found

2-(2-Ethoxyethoxy)ethanol

Measured: 5.72×10^{-11}

Predicted: 3.59×10^{-11}

Image not found

Propane, 2,2-diethoxy-

Measured: 1.17×10^{-11}

Predicted: 1.60×10^{-11}